Theory of Local Density of States of $d_{x^2-y^2}$-Wave Superconducting State Near the Surfaces of the t-J Model

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Spatial dependencies of the pair potential and the local density of states near the surfaces of $d_{x^2-y^2}$-wave superconductors are studied theoretically. The calculation is based on the t-J model within a mean-field theory with Gutzwiller approximation. Various types of surface geometries are considered. Similar to our result in the extended Hubbard model, it is found that the formation of zero-energy states strongly depends on the surface geometry. In addition to this feature, the zero-energy states give peak splitting for the (110) surfaces when the super-exchange interaction J is large. This is due to the induced s-wave component near the surface. The present result explains the microscopic origin of the spontaneous time-reversal symmetry breaking at the surfaces of high-T_c superconductors.

The t-J model[1] is believed to explain the phase diagram of high-T_c materials including the so-called pseudogap above T_c and thus is a realistic model for high-T_c superconductors.[2] Although there are many works regarding this model, the quasiparticle properties in nonuniform systems including surfaces or interfaces are not clear at this stage except for those in the case with a vortex.[3] Since $d_{x^2-y^2}$-wave pair potential is the most promising symmetry in the t-J model for actual doping concentrations, we expect an interference effect of the quasiparticle due to the sign-change of the pair potential[4] at the surface.

Recent theoretical works within quasiclassical approximation revealed a novel interference effect peculiar to the unconventional superconductivity.[5,6,7,8,9,10,11] One of the interesting interference effects is the appearance of zero-energy states (ZES) at the surface, which is due to the sign-change of pair potential when the quasiparticles are reflected at the surface.[7] This localized ZES manifests itself as a zero-bias conductance peak (ZBCP) in tunneling experiments.[5,12] A recent experiment

using a well-oriented (110) surface detects a ZBCP.[13] However this ZBCP is often not detected experimentally, which indicates that the presence of ZBCP strongly depends on the surface quality. One of the main purposes of the present letter is to clarify the origin of this dependence on the subtle difference of the surface in the t-J model.

Another interesting feature is the splitting of ZBCP which was observed in recent experiments.[12, 14] This splitting is considered to be due to the coexistence of a s-wave pair potential induced near the surface. Till date, theories[15, 16, 17] have assumed an additional attractive potential which favors the s-wave component. For example, Fogelström et $al.$[15] suggested electron-phonon interaction as an origin of the s-wave component. However, in this letter, we will show that the t-J model automatically induces the s-wave component near the surface and thus gives a natural explanation of the splitting of ZBCP. We discuss the doping and J/t dependence of this splitting.

Although the previous theories[5, 6, 7, 8, 9, 10, 11, 15, 16, 17, 18, 19] clarified some important properties of high-T_c superconductors, they ignored several distinctive features characteristic to high-T_c materials: i) short coherence length, which invalidates the quasiclassical approximation and ii) strong correlation. In order to deal with the effect of short coherence length, Tanuma et $al.$[20] developed local density of states (LDOS) theory based on the extended Hubbard model beyond quasiclassical approximation. They clarified that LDOS of the $d_{x^2-y^2}$-wave superconductor is sensitive to the atomic structures near the surface. However, the strong correlation effect is not sufficiently considered in their approach.

To consider this problem, we develop a theory of the t-J model near the surface.[21] By using this model, we can naturally treat the d-wave superconductivity with short coherent length and strong correlation. The merit of studying the t-J model is that we can systematically investigate the doping or Fermi surface dependence which can be directly compared with the experimental results. In this letter, the LDOS of quasiparticles is obtained based on the self-consistently determined pair potential. Since it is difficult to treat the constraint in the t-J model analytically, we apply the Gutzwiller approximation.[22] The validity of this method was verified by comparing the variational energies of the bulk states with those obtained in the variational Monte Carlo method.[23] After the Gutzwiller approximation, the spatial dependence of the pair potential is determined self-consistently within the mean-field approximation as in our previous work regarding vortex core.[3]

The t-J model is given as[1]

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle, \sigma} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$
$$- \mu \sum_{i,\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}, \tag{1}$$

where J and $\boldsymbol{S}_i$ are the super-exchange interaction and the spin-1/2 operator at the i-th site, respectively. Here $\langle i, j \rangle$ stands for the summation over the nearest-neighbor pairs. The operator $\tilde{c}_{i\sigma} = c_{i\sigma} P_G$ with the Gutzwiller projection operator $P_G = \Pi_i (1 - n_{i\uparrow} n_{i\downarrow})$ excludes the double

occupancy. We use the Gutzwiller approximation[22] in which the effect of the projection is taken into account as statistical weights. The expectation values are estimated as

$$\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle = g_t \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle_0,$$

$$\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = g_s \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle_0, \tag{2}$$

where $\langle \cdots \rangle$ and $\langle \cdots \rangle_0$ represent the expectation values in terms of a Gutzwiller-type variational wave function $P_G|\Phi\rangle$ and a BCS wave function, $|\Phi\rangle$, respectively. The renormalized coefficients $g_t = 2\delta/(1+\delta)$ and $g_s = 4/(1+\delta)^2$ with the hole concentration $\delta(= 1-n)$ are determined from the probabilities of involved configurations.[22,23] Using this approximation, eq. (1) can be transformed into

$$\mathcal{H}_{\mathrm{eff}} = -t_{\mathrm{eff}} \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}) + J_{\mathrm{eff}} \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{3}$$

$$t_{\mathrm{eff}} = g_t t, \quad J_{\mathrm{eff}} = g_s J. \tag{4}$$

In this letter, we consider various types of boundaries as shown in Fig. 1. The index m in Fig. 1(d) denotes the period of zigzag structures, and we will show that the LDOS strongly depends on this period. The case of $m = 0$ [$m = 1$] corresponds to a flat (100) [(110)] surface shown in Fig. 1(a) [(b)]. In the following, we discuss the cases with $m = 0, 1$ and 2.

For this model, we perform a mean-field approximation with site-dependent pair potential Δ_{ij} and Hartree-Fock parameter $\xi_{ij\sigma}$,

$$\Delta_{ij} = \frac{3}{4} J_{\mathrm{eff}} \langle c_{i\uparrow} c_{j\downarrow} \rangle, \quad \xi_{ij\sigma} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle. \tag{5}$$

Here we have assumed $\xi_{ij\uparrow} = \xi_{ij\downarrow} = \xi_{ij}$. For simplicity ξ_{ij} and μ are fixed to the values ξ_0 and μ_0 determined in the bulk without boundaries. We use periodic boundary conditions in the y-direction and open boundary conditions in the x-direction. Furthermore, we assume that Δ_{ij} is translationally invariant in the tangential direction along the surface. Thus, the unit cell is $N_L \times 1$, with N_L being the number of sites in the x-direction. After Fourier transformation, the mean-field Hamiltonian becomes

$$\mathcal{H}_{\mathrm{eff}} = \sum_{k_y, i, j} \begin{pmatrix} C_{i\uparrow}^{\dagger}(k_y) & C_{i\downarrow}(-k_y) \end{pmatrix} \begin{pmatrix} \hat{H}_{ij}(k_y) & \hat{\Delta}_{ij}(k_y) \\ \hat{\Delta}_{ji}^{\dagger}(k_y) & -\hat{H}_{ji}(-k_y) \end{pmatrix} \begin{pmatrix} C_{j\uparrow}(k_y) \\ C_{j\downarrow}^{\dagger}(-k_y) \end{pmatrix} \tag{6}$$

with

$$\hat{H}_{ij}(k_y) = -\sum_{\pm} [(t_{\mathrm{eff}} + \frac{3}{4} J_{\mathrm{eff}} \xi_0)(\delta_{i,j\pm1} + e^{\mp i k_y a} \delta_{i,j\pm m})] - \mu_0 \delta_{i,j}, \tag{7}$$

$$\hat{\Delta}_{ij}(k_y) = \sum_{\pm} [\Delta_{ij,x} \delta_{i,j\pm1} + \Delta_{ij,y} e^{\mp i k_y a} \delta_{i,j\pm m}], \tag{8}$$

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where $C_{j\sigma}(k_y)$ is the Fourier transformed form of $c_{j\sigma}$ with respect to the surface direction and j is now the site number in the x-direction ($j = 1, \cdots, N_L$). The wave vector k_y changes from $-\pi/a$ to π/a. In the above, a is the lattice constant and we use $N_L = 300$. The above Hamiltonian is diagonalized by Bogoliubov transformations[24, 25] given as $C_{j\uparrow}^\dagger(k_y) = \sum_\nu \gamma_\nu^\dagger(k_y)\mathcal{U}_{j,\nu}^*$, and $C_{i\downarrow}(-k_y) = \sum_\nu \gamma_\nu^\dagger(k_y)\mathcal{U}_{N_L+i,\nu}^*$. The spatial dependence of the pair potential is determined self-consistently as

$$\Delta_{j\pm m,j,y} = \frac{3}{4}J_{\text{eff}}\sum_{k_y,\nu}\mathcal{U}_{j,\nu}\mathcal{U}_{N_L+j\pm m,\nu}^*\{1 - f(E_\nu(k_y))\}e^{\pm ik_y a}, \tag{9}$$

$$\Delta_{j\pm 1,j,x} = \frac{3}{4}J_{\text{eff}}\sum_{k_y,\nu}\mathcal{U}_{j,\nu}\mathcal{U}_{N_L+j\pm 1,\nu}^*\{1 - f(E_\nu(k_y))\}. \tag{10}$$

where $\Delta_{j\pm m,j,y}$ and $\Delta_{j\pm 1,j,x}$ are the pair potentials along the y-axis and x-axis directions, respectively. The above $f(E_\nu(k_y))$ denotes the Fermi distribution function.

We solve the effective Hamiltonian in Eq. (6) by numerical diagonalization and carry out an iteration until the pair potentials $\Delta_{i,j,x}$ and $\Delta_{i,j,y}$ are determined self-consistently. The obtained equations are decomposed into real and imaginary parts as

$$\Delta_{\text{R},j,x(y)} \equiv \text{Re}(\Delta_{ij,x(y)})/\Delta_0,$$
$$\Delta_{\text{I},j,x(y)} \equiv \text{Im}(\Delta_{ij,x(y)})/\Delta_0. \tag{11}$$

Figure 2(b) shows the calculated results of the spatial dependence of the pair potential for the flat (110) surface for $J/t = 0.4$ and $\delta = 0.15$. For this geometry, $\Delta_{\text{R},j,x(y)}$ and $\Delta_{\text{I},j,x(y)}$ can be regarded as d-wave and extended s-wave components of the pair potential, respectively. The quantity $\Delta_{\text{R},j,x(y)}$ is suppressed at the surface and increases monotonically as we approach the middle of the lattice. This behavior is consistent with the quasiclassical theory.[19] The extended s-wave component is induced near the surface, whose magnitude is about 30% relative to the bulk d-wave component. We find an atomic-scale spatial oscillation of the s-wave component, which is completely neglected in the quasiclassical approximation.

Using the self-consistently determined pair potential, we calculate the LDOS at every site. In order to compare our theory with scanning tunneling microscopy (STM) experiments, we assume that the STM tip is metallic with a flat density of states, and that the tunneling probability is finite only for the nearest site from the tip. The LDOS at i-th site is given as,

$$\rho_i \sim \int_{-\infty}^\infty d\omega \rho_i(\omega)\text{sech}^2(\frac{\omega + E}{2k_B T}), \tag{12}$$

$$\rho_i(\omega) = -\frac{2}{\pi}\text{Im}\sum_k G_i^R(k,\omega)$$

$$= 2\sum_k \sum_\nu |\mathcal{U}_{i,\nu}|^2\delta(\omega - E_\nu(\boldsymbol{k})) \tag{13}$$

where $G_i^R(k,\omega)$ is the Fourier component of the retarded Green's function with energy ω. In the actual STM experiments, since the magnitude of the transparency between the tip and surface is

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small, the tunneling conductance converges to the normalized LDOS

$$\bar{\rho}(E) = \frac{\displaystyle\int_{-\infty}^{\infty} d\omega \rho_{i,S}(\omega)\mathrm{sech}^2(\frac{\omega + E}{2k_B T})}{\displaystyle\int_{-\infty}^{\infty} d\omega \rho_N(\omega)\mathrm{sech}^2(\frac{\omega + 2\Delta_0}{2k_B T})}, \tag{14}$$

at low temperatures,[6] where $\rho_{i,S}(\omega)$ denotes the LDOS in the superconducting state and $\rho_N(\omega)$ denotes the LDOS in the normal state. In this letter, $\rho_N(\omega)$ is obtained from the LDOS at the $N_L/2$-th site away from the boundary.

Figure 2(c) shows the calculated LDOS for various sites near the flat (110) surface. This zero-energy peak (ZEP) is the manifestation of ZES, which are formed due to the sign-change of the $d_{x^2-y^2}$-wave pair potential. A remarkable difference between the present results and those based on the quasiclassical theory is seen in the oscillatory behaviors of the LDOS.[10] This oscillation can be regarded as the Friedel oscillation, the period of which is the inverse of the Fermi momentum. Furthermore, we find that the ZEP of the LDOS is split into two at all sites near the surface (see Fig. 2(c)). The splitting of the ZBCP in tunneling spectra is also obtained in the quasiclassical approximation.[16, 15] Its origin is the s-wave component induced near the surface which blocks the motion of quasiparticles near the (110) surface.[3, 16] In effect, the splitting is not visible when J/t is decreased and the amplitude of the induced imaginary component is small. On the other hand, when δ is increased, the splitting becomes larger. This is because $\Delta_{\mathrm{R},j,x(y)}$ is reduced in magnitude with the increase of δ, while $\Delta_{\mathrm{I},j,x(y)}$ is insensitive to the change of δ. Recently, experimental observations of the peak splitting are reported in the tunneling spectroscopy of high-T_c superconductors.[12, 14] This indicates that the s-wave component is induced near the sample surface and the spontaneous time-reversal symmetry breaking actually takes place in high-T_c superconductors.

We also study the flat (100) surface shown in Fig. 1(a). In this case, $\Delta_{\mathrm{I},j,x(y)}$ is not induced near the surface. Since the quasiparticles do not feel the sign-change of the pair potential at the (100) surface, the ZEP do not appear.

Next, we discuss the case of a 1×2 zigzag surface (see Fig. 3(a)). The obtained pair potential has complex spatial dependence as compared to the cases with (100) and (110) surfaces. The quantity $\Delta_{\mathrm{I},j,x(y)}$ is not induced as shown in Fig. 3(b). On the other hand, $\Delta_{\mathrm{R},j,x(y)}$ has an oscillation and behaves like a $d_{x^2-y^2}$ pair potential far away from the boundary. The complex spatial dependencies of the pair potential reflect on the LDOS as an anomalous structure with many dips and peaks (see Fig. 3(c)). It should be noted that the ZES are not formed near the surface. A similar property was also obtained on the 1×2 zigzag surface in the extended Hubbard model.[26] The reason for the absence of ZEP is as follows. The wave function of ZES spatially oscillates with the period of the inverse of the Fermi momentum as discussed in the (110) surface.[15, 16, 17] In the underdoped region, since the Fermi surface is nearly square, the period of the oscillation of the wave function is roughly coincident with $2a$. Consequently, the node and the antinode appear alternatively. However, for

the 1×2 zigzag structure the phase of node and antinode does not coincide. This disappearance of the ZES can be regarded as an interference effect of the standing-wave, which cannot be explained by means of the quasiclassical theory.

In this letter, we have investigated the LDOS near the surfaces of the $d_{x^2-y^2}$-wave superconductor based on the t-J model within the Gutzwiller approximation. In the present calculation, the non-local feature of the pair potential and the atomic-scale geometry of the surface are explicitly taken into account. The present result gives a microscopic basis for the spontaneous time-reversal symmetry breaking in $d_{x^2-y^2}$-wave superconductors where the s-wave component is induced as the $d + is$ state near the surface. It is clarified that when the amplitude of the induced s-wave component is enhanced with the increase of the magnitude of J, the ZEP of LDOS is split into two.
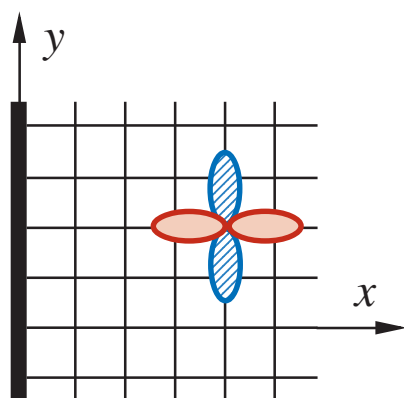
[1] F.C. Zhang and T.M. Rice: Phys. Rev. B **37** (1988) 3759.

[2] H. Fukuyama and H. Kohno: Physica C **282-287** (1997) 124.

[3] A. Himeda, M. Ogata, Y. Tanaka, and S. Kashiwaya: J. Phys. Soc. Jpn. **66** (1997) 3367.

[4] D.J. Van Harlingen: Physica C **282-287** (1997) 128.

[5] S. Kashiwaya, Y. Tanaka, M. Koyanagi, H. Takashima, and K. Kajimura: Phys. Rev. B **51** (1995) 1350.

[6] S. Kashiwaya, Y. Tanaka, M. Koyanagi, and K. Kajimura: Phys. Rev. B **53** (1996) 2667.

[7] C.R. Hu: Phys. Rev. Lett. **72** (1994) 1526.

[8] Y. Tanaka and S. Kashiwaya: Phys. Rev. Lett. **74** (1995) 3451; Phys. Rev. B **53** (1996) 9371.

[9] Y. Tanaka and S. Kashiwaya: Phys. Rev. B **53** (1996) R11957; Phys. Rev. B **56** (1997) 892.

[10] M. Matsumoto and H. Shiba: J. Phys. Soc. Jpn. **64** (1995) 1703.

[11] Yu. Barash, A.A. Svidzinsky, and H. Burkhardt: Phys. Rev. B **55** (1997) 15282.

[12] M. Covington, M. Aprili, L.H. Greene, F. Xu, and C.A. Mirkin: Phys. Rev. Lett. **79** (1997) 277.

[13] L. Alff, H. Takashima, S. Kashiwaya, N. Terada, H. Ihara, Y. Tanaka, M. Koyanagi, and K. Kajimura: Phys. Rev. B **55** (1997) 14757.

[14] S. Kashiwaya, Y. Tanaka, N. Terada, M. Koyanagi, S. Ueno, L. Alff, H. Takashima, Y. Tanuma, and K. Kajimura: to be published in J. Phys. Chem. Solid.

[15] M. Fogelström, D. Rainer, and J.A. Sauls: Phys. Rev. Lett. **79** (1997) 281.

[16] M. Matsumoto and H. Shiba: J. Phys. Soc. Jpn. **65** (1995) 3384; *ibid.* **65** (1995) 4867.

[17] M. Sigrist, K. Kuboki, P.A. Lee, A.J. Millis, and T.M. Rice: Phys. Rev. B **53** (1996) 2835.

[18] L.J. Buchholtz, M. Palumbo, D. Rainer, and J.A. Sauls: J. Low. Temp. Phys. **101** (1995) 1079; *ibid.* **101** (1995) 1099.

[19] Y. Nagato and K. Nagai: Phys. Rev. B **51** (1995) 16254.

[20] Y. Tanuma, Y. Tanaka, M. Yamashiro, and S. Kashiwaya: Physica C **282-287** (1997) 1857; to be published in

Phys. Rev. B. **57** (1998).

[21] M. Ogata, unpublished.

[22] F.C. Zhang, C. Gross, T.M. Rice, and H. Shiba: Supercond. Sci. Technol. **1** (1988) 36.

[23] H. Yokoyama and M. Ogata: J. Phys. Soc. Jpn. **65** (1996) 3615.

[24] M. Tachiki, S. Takahashi, F. Steglich, and H. Adrian: Z. Phys. B, **80** (1990) 161.

[25] O. Sato, Y. Tanaka, and A. Hasegawa: J. Phys. Soc. Jpn. **61** (1992) 2640.

[26] Y. Tanuma, Y. Tanaka, M. Yamashiro, and S. Kashiwaya: *Advances in superconductivity IX, Springer-Verlag Tokyo 1997*, 307.
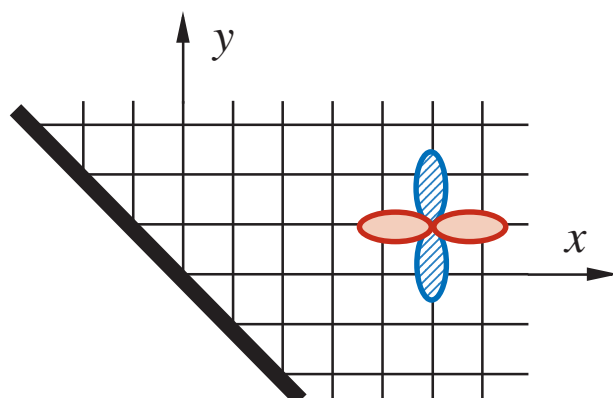
Fig. 1. Schematic illustration corresponding to $1 \times m$ zigzag surface : (a) a flat (100) surface ($m = 0$), (b) a flat (110) surface ($m = 1$), (c) a 1×2 zigzag surface ($m = 2$) and (d) a $1 \times m$ zigzag surface.

Fig. 2. (a) Schematic illustration of a flat (110) surface, (b) the spatial dependence of the normalized pair potential and (c) the local density of states for $J/t = 0.4$ and $\delta = 0.15$ ($\Delta_0/t = 0.105$).

Fig. 3. (a) Schematic illustration of a 1×2 zigzag surface, (b) the spatial dependence of the normalized pair potential and (c) the local density of states for $J/t = 0.2$ and $\delta = 0.1$ ($\Delta_0/t = 0.054$).

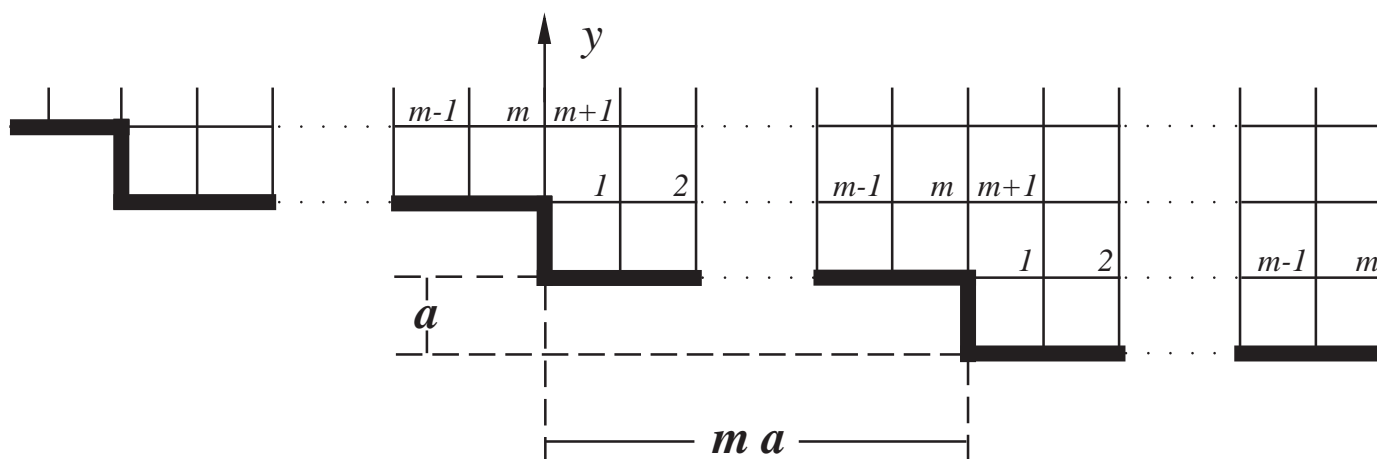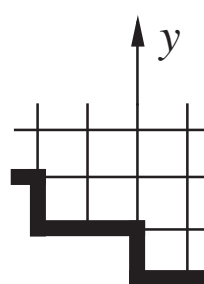(a)

(b)

(d)

(a)

R

P

Q

Flat (110) surface

(b)

$\Delta_{ij,x(y)} / \Delta_0$

1

0

-1

Normalized pair potential

$\Delta_{R,j,x}$

$\Delta_{I,j,x} = \Delta_{I,j,y}$

$\Delta_{R,j,y}$

P Q R

0 5 10 15

Number of lattice sites

(c)

$\bar{\rho}(E)$

Normalized Local Density Of States

P
Q
R

$J/t=0.4$
$\delta=0.15$

10

0

-1 0 1

Normalized Energy

$E / 2\Delta_0$

(a) Q R P 1×2 zigzag surface

(b) $\Delta_{ij,x(y)} / \Delta_0$ — Normalized pair potential

$\Delta_{R,j,x}$

Δ_I

$\Delta_{R,j,y}$

P Q R

Number of lattice sites

(c) $\bar{\rho}(E)$ — Normalized Local Density Of States

P
Q
R

$J/t = 0.2$
$\delta = 0.10$

Normalized Energy $E / 2\Delta_0$